

REMARKS

Applicants respectfully request reconsideration and further examination of the present application.

I. Status of Pending Claims

In this Amendment B, claims 54 and 102 have been amended and claims 111-114 have been added to more particularly claim certain embodiments of the present invention. Specifically:

Claim 54 has been amended to more clearly indicate that the ratio recited therein ranges from 0.2:1 to 0.8:1. Support for this amendment may be found in original claim 54, as well as in the specification on, for example, page 13, lines 3-20.

Claim 102 has been amended to more clearly indicate that the hydrophobic polymer layer referenced therein has a minimum thickness such that, upon being subjected to the conditions recited therein, the thickness of the polymer layer, of which the hydrophobic polymer layer is a part, is reduced by less than about 40%. Support for this amendment may be found in the specification on, for example, page 12, lines 9-20.

Finally, claims 111-114 have also been added, with one or more of these claims specifying, for example, (i) that the hydrophobic polymer chains of the hydrophobic polymer layer are covalently attached to the substrate surface, and/or (ii) that an end of each of the hydrophilic polymer chains of the hydrophilic layer are covalently attached to a hydrophobic polymer chain. Support for these new claims may be found in the present application, for example, on page 12, lines 9-20, page 21, lines 4-9, and page 25, lines 2-5.

Accordingly, claims 49-62, 64-69 and 102-114 are now pending.

II. **35 U.S.C. §102(e)**

Reconsideration is respectfully requested of the rejection of claims 49-62, 64-69 and 102-110 as being anticipated by Wagner et al. (U.S. Patent No. 6,475,808).

A. *Claims 49-62 and 64-69*

Claim 49, from which claims 50-62 and 64-69 depend, is directed to a polymer brush for binding a molecule in an aqueous sample in an assay. The brush comprises:

a substrate surface, **a hydrophobic layer** comprising hydrophobic polymer chain segments attached to the substrate surface and **having a dry thickness of at least about 50 angstroms**, and a hydrophilic layer attached to the hydrophobic layer containing functional groups for the attachment of a probe for binding the molecule. (emphasis added)

The Office asserts that the claims of Wagner et al. *per se* describe/anticipate claim 49, as well as the claims depending therefrom. In this regard it is noted that the Wagner et al. patent contains three claims. Claim 1 is directed, in relevant part, to a device comprising a substrate, a hydrophobic monolayer formed of alkyl chains chemisorbed or physisorbed to the substrate surface, and a hydrophilic monolayer formed from hydrophilic chains, the ends of which are covalently linked to the ends of alkyl chains. Claim 2 depends from claim 1 and further specifies that the hydrophobic polymer chains are hydrocarbon chains having a length of 8-22 carbon atoms. Claim 3 depends from claim 1 and further specifies that the hydrophilic polymer chains are polyethylene glycol chains.

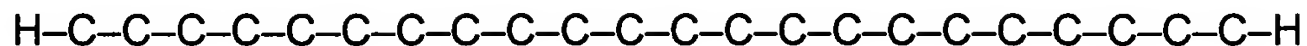
Consistent with the Office's exclusive reliance on the claims of Wagner et al., Applicants note that Wagner et al. provide no specific reference, either in the detail description or the working examples, to a device as claimed. That is, with the exception of the claims, Wagner et al. fail to specifically reference a device having a hydrophobic polymer layer present on a substrate surface, and a hydrophilic polymer layer present on the hydrophobic polymer layer.

With respect to the claims of Wagner et al., Applicants submit that each and every element of Applicants' claims is not disclosed. Furthermore, as Applicants previously stated (see Applicants' Amendment A), the mere fact that a certain result or characteristic may occur or be present is not sufficient to establish the inherency of that result or characteristic. See MPEP §2112 (citing *In re Rijckaert*, 9 F.3d 1531, 1534 (Fed. Cir. 1993)). Rather, the allegedly inherent characteristic must necessarily flow from the teachings of the applied prior art. See MPEP §2112 (citing *Ex parte Levy*, 17 USPQ2d 1461, 1464 (Bd. Pat. App. & Inter. 1990)). This is simply not the case here.

As noted above, pending claim 49 is directed to a polymer brush that includes a hydrophobic polymer layer having a dry thickness of at least 50 angstroms. In comparison, Wagner et al. provide no details that relate to the thickness of their hydrophobic polymer layer in claim 1. Claim 2, however, provides compositional details of this polymer layer, indicating that the hydrophobic polymer chains are hydrocarbon chains, and thus contain only hydrogen and carbon atoms. Additionally, claim 2 states that these hydrocarbon chains have a length of 8-22 carbon atoms.

Applicants respectfully submit that a hydrocarbon chain of 8-22 carbon atoms in length would not inherently have a length of at least 50 angstroms. Rather, based on the commonly recognized bond lengths of (i) 1.09 angstroms for a C-H bond, and (ii) 1.53 angstroms for a C-C bond, Applicants respectfully submit that a hydrocarbon chain having 22 carbon atoms, as illustrated below (wherein only the terminal C-H bonds are

shown, given that these are the only two of such bonds that would possibly add to the total length of the chain):



would have a theoretical maximum length of only approximately 34.31 angstroms (i.e., 21 C-C bonds * 1.53 angstroms per bond = 32.13 angstroms, plus 2 C-H bonds * 1.09 per bond = 2.18 angstroms, for a total length of 34.31 angstroms).¹

Additionally, Applicants respectfully submit the disclosure by Wagner et al. is not a sufficient basis upon which to conclude the presently claimed invention is disclosed, either explicitly or inherently, because Wagner et al. is non-enabling for the invention being claimed therein. More specifically, Applicants submit that Wagner et al. do not enable the device of claims 1-3, given that Wagner et al. provide no specific discussion or illustration related to the preparation of a device comprising a substrate, a hydrophobic monolayer formed of alkyl chains chemisorbed or physisorbed to the substrate surface, and a hydrophilic monolayer formed from hydrophilic chains, the ends of which are covalently linked to the ends of alkyl chains. In as much as the disclosure in an assertedly anticipating reference must be adequate to enable possession of the subject matter being relied upon, and furthermore given that such is not the case here, Applicants submit the present rejection is improper.²

In view of the foregoing, claim 49 is submitted as novel over the cited reference. Accordingly, Applicants respectfully request reconsideration of the rejection of this claim. In as much as claims 50-63 and 64-69, as well as new claims 111 and 112, depend from claim 49, these claims are submitted as novel over the cited reference for at least the same reasons as those noted with respect to claim 49. Additionally, (i) claims 50-52 are submitted as novel over the cited reference because, as noted above,

¹ See, e.g., Table 1.5 from Advanced Organic Chemistry, J. March ed., (1992), which is attached hereto as Exhibit A.

² See, e.g., *Elan Pharmaceuticals, Inc. v. Mayo Foundation for Medical Education and Research*, 346 F.3d 1051, 1055 (Fed. Cir. 2003).

Wagner et al. do not disclose any details regarding the size of the hydrophilic polymer, and thus do not disclose a polymer brush wherein the hydrophobic layer has a dry thickness of at least about 100, 1000 or 2000 angstroms, respectively, while (ii) claims 56 and 57 are submitted as novel over the cited reference because, as noted above, Wagner et al. do not disclose a polymer brush wherein the hydrophilic polymer has a molecular weight of at least 1000, or between at least 1000 and less than 5,000,000, respectively. Finally, new claims 111 and 112 are submitted as novel over Wagner et al., in as much as these claims specify the covalent attachment of the hydrophobic polymer chains to the substrate surface, and the covalent attachment of the hydrophilic polymer chains to the hydrophobic polymer chains.

B. Claims 102-110

Claim 102, from which claims 103-110 depend, is directed to a polymer brush for binding a molecule in an aqueous sample in an assay. The polymer brush comprises:

a substrate surface having a polymer layer thereon, said polymer layer comprising a first hydrophobic layer attached to the substrate surface, and a second hydrophilic layer attached to the hydrophobic layer containing groups for the attachment of a probe for binding the molecule, said brush being characterized in that said **hydrophobic polymer layer has a minimum thickness** such that, upon being immersed in a 10 mmolar sodium hydroxide solution for about 15 minutes, the polymer layer thickness is reduced by less than about 40%. (emphasis added)

As Applicants previously noted (see Applicants' Amendment A, as well as page 12, lines 9-20 of the present application), Applicants discovered that the stability of the attachment of the polymer chains to the substrate surface of the brush, when exposed to hydrolyzing conditions, can be increased by forming a hydrophobic layer of some

minimum thickness on the substrate surface. This hydrophobic layer thus acts as a "barrier" which limits access of hydrolyzing reactants to these covalent bonds. As a result, the degree to which the thickness of the polymer layer on the substrate surface is reduced by these hydrolyzing conditions is limited.

Applicants respectfully submit the disclosure by Wagner et al. is not a sufficient basis upon which to conclude the presently claimed invention is disclosed, either explicitly or inherently, because Wagner et al. is non-enabling for the invention being claimed therein. More specifically, Applicants respectfully submit that Wagner et al. do not enable the device of claims 1-3, given that Wagner et al. provide no specific discussion or illustration related to the preparation of a device comprising a substrate, a hydrophobic monolayer formed of alkyl chains chemisorbed or physisorbed to the substrate surface, and a hydrophilic monolayer formed from hydrophilic chains, the ends of which are covalently linked to the ends of alkyl chains. In as much as the disclosure in an assertedly anticipating reference must be adequate to enable possession of the subject matter being relied upon, and furthermore given that such is not the case here, Applicants submit the present rejection is improper.

In view of the foregoing, claim 102 is submitted as novel over the cited reference. Accordingly, Applicants respectfully request reconsideration of the rejection this claim. In as much as claims 103-110, as well as new claims 113 and 114, depend from claim 102, these claims are submitted as novel over the cited reference for at least the same reasons as those noted with respect to claim 102. Additionally, claims 105 and 106 are submitted as novel over the cited reference because, as noted above, Wagner et al. do not disclose a polymer brush wherein the hydrophobic layer has a dry thickness of at least about 100 or 1000 angstroms, respectively. Finally, new claims 113 and 114 are submitted as novel over Wagner et al., in as much as these claims specify the covalent attachment of the hydrophobic polymer chains to the substrate surface, and the covalent attachment of the hydrophilic polymer chains to the hydrophobic polymer chains.

III. 35 U.S.C. §102(e)/§103

Reconsideration is respectfully requested of the rejection of claims 49-62, 64-69 and 102-110 as being anticipated by, or obvious in view of, each of Klaerner et al. (U.S. Publication No. 2002/0001845) or Klaerner et al. (U.S. Patent No. 6,833,276, hereinafter). In this regard it is to be noted that the published application cited here ultimately matured into the 6,833,276 patent. Accordingly, both references will be collectively referred to hereinafter as "Klaerner et al."

A. §102(e)

As noted above, claim 49, from which claims 50-62 and 64-69 depend, is directed to a polymer brush for binding a molecule in an aqueous sample in an assay. The brush comprises:

a substrate surface, a **hydrophobic layer** comprising hydrophobic polymer chain segments attached to the substrate surface and **having a dry thickness of at least about 50 angstroms**, and a hydrophilic layer attached to the hydrophobic layer containing functional groups for the attachment of a probe for binding the molecule. (Emphasis added)

Also as noted above, claim 102, from which claims 103-110 depend, is directed to a polymer brush for binding a molecule in an aqueous sample in an assay. The polymer brush comprises:

a substrate surface having a polymer layer thereon, said polymer layer comprising a first hydrophobic layer attached to the substrate surface, and a second hydrophilic layer attached to the hydrophobic layer containing groups for the

attachment of a probe for binding the molecule, said brush being characterized in that said **hydrophobic polymer layer has a minimum thickness** such that, upon being immersed in a 10 mmolar sodium hydroxide solution for about 15 minutes, the polymer layer thickness is reduced by less than about 40%. (Emphasis added)

The Office asserts that the cited references describe a polymer brush comprised of a substrate to which is attached a hydrophobic polymer, upon which a functionalized hydrophilic polymer is layered. The Office further asserts that the brush of Klaerner et al. anticipates the brush of claims 49-62, 64-69 and 102-110.

Applicants acknowledge that Klaerner et al. disclose the possibility of a polymer brush having polymer chains attached to a substrate surface wherein a hydrophobic segment is present between the substrate surface and the water-soluble or water-dispersible segment (see, e.g., column 11, lines 6-16). Applicants further acknowledge that Klaerner et al. disclose that the polymer layer on the substrate surface has a determinable thickness, ranging for example from about 20 to about 2000 angstroms (see, e.g., column 28, lines 54-62). Notably, however, Klaerner et al. fail to disclose a polymer brush wherein the hydrophobic layer, specifically, has a dry thickness of at least about 50 angstroms. Klaerner et al. also fail to disclose a polymer brush wherein the hydrophobic layer, specifically, has a minimum thickness such that, upon being immersed in a 10 mmolar sodium hydroxide solution for about 15 minutes, the polymer layer thickness is reduced by less than about 40%. In fact, Klaerner et al. make no reference specifically to the thickness of any hydrophobic layer, nor do they prepare in any working example a brush which includes a hydrophobic polymer layer on the substrate surface, between the substrate surface and the water-soluble or water-dispersible polymer segments.

In view of the foregoing, Applicants submit that each and every element of Applicants' claims is not disclosed. Furthermore, as Applicants stated above, the mere

fact that a certain result or characteristic may occur or be present is not sufficient to establish the inherency of that result or characteristic. See MPEP §2112 (citing *In re Rijckaert*, 9 F.3d 1531, 1534 (Fed. Cir. 1993)). Rather, the allegedly inherent characteristic must necessarily flow from the teachings of the applied prior art. See MPEP §2112 (citing *Ex parte Levy*, 17 USPQ2d 1461, 1464 (Bd. Pat. App. & Inter. 1990)). This is simply not the case here.

In view of the foregoing, claim 49 is submitted as novel over Klaerner et al. Accordingly, Applicants respectfully request reconsideration of the rejection this claim. In as much as claims 50-63 and 64-69, as well as new claims 111 and 112, depend from claim 49, these claims are submitted as novel over the cited reference for at least the same reasons as those noted with respect to claim 49. Additionally, claims 50-52 are submitted as novel over the cited reference because, as noted above, Klaerner et al. do not disclose a polymer brush wherein the hydrophobic layer, specifically, has a dry thickness of at least about 100, 1000 or 2000 angstroms, respectively.

In view of the foregoing, claim 102 is also submitted as novel over Klaerner et al. Applicants therefore respectfully request reconsideration of the rejection this claim, as well. In as much as claims 103-110, as well as new claims 113 and 114, depend from claim 102, these claims are submitted as novel over the cited reference for at least the same reasons as those noted with respect to claim 102. Additionally, claims 105 and 106 are submitted as novel over the cited reference because, as noted above, Klaerner et al. do not disclose a polymer brush wherein the hydrophobic layer, specifically, has a dry thickness of at least about 100 or 1000 angstroms, respectively.

B. §103

Applicants wish to invoke the §103(c) exception to establish that the Klaerner et al. references cited herein above may not be used as §103 prior art against the present application. In the context of rejections under §102(e) and/or §103(a), the following is to be noted:

Effective November 29, 1999, subject matter which was prior art under former 35 U.S.C. 103 via 35 U.S.C. 102(e) is now disqualified as prior art against the claimed invention if that subject matter and the claimed invention "were, at the time the invention was made, owned by the same person or subject to an obligation of assignment to the same person." (MPEP 706.02(I)(1), first paragraph.)

In order to be disqualified as prior art under 35 U.S.C. 103(c), the subject matter which would otherwise be prior art to the claimed invention and the claimed invention must be commonly owned at the time the claimed invention was made. (MPEP 706.02(I)(2), first paragraph.)

Applicants would like to establish common ownership at this time: Application No. 09/911,683 to Klaerner et al., which published as U.S. Publication No. 2002/ 0001845 on January 3, 2002 and which ultimately matured into U.S. Patent No. 6,833,276, was, at the time the invention of the present application (Application No. 10/043,394) was made, owned by Symyx Technologies, Inc., Santa Clara, CA (US).

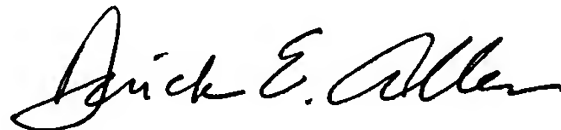
In view of the foregoing, Applicants respectfully request withdrawal of the present rejection of pending claims 49-62, 64-69 and 102-110.

CONCLUSION

In view of the foregoing, favorable reconsideration and allowance of all pending claims is respectfully requested.

The Commissioner is hereby authorized to charge any underpayment and credit any overpayment of government fees to Deposit Account No. 19-1345.

Respectfully submitted,



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electronegativity, such as Si,⁴³ Mg, etc., and perhaps alkyl groups. Alkyl groups⁴⁴ were formerly regarded as electron-donating, but many examples of behavior have been found that can be interpreted only by the conclusion that alkyl groups are electron-withdrawing compared with hydrogen.⁴⁵ In accord with this is the value of 2.472 for the group electronegativity of CH₃ (Table 1.2) compared with 2.176 for H. We shall see that when an alkyl group is attached to an unsaturated or trivalent carbon (or other atom), its behavior is best explained by assuming it is $+I$ (see, for example, pp. 168, 176, 270, 511), but when it is connected to a saturated atom, the results are not as clear, and alkyl groups seem to be $+I$ in some cases and $-I$ in others⁴⁶ (see also p. 271). Similarly, it is clear that the field-effect order of alkyl groups attached to unsaturated systems is tertiary > secondary > primary > CH₃, but this order is not always maintained when the groups are attached to saturated systems. Deuterium is electron-donating with respect to hydrogen.⁴⁷ Other things being equal, atoms with sp bonding generally have a greater electron-withdrawing power than those with sp^2 bonding, which in turn have more electron-withdrawing power than those with sp^3 bonding.⁴⁸ This accounts for the fact that aryl, vinylic, and alkynyl groups are $-I$. Field effects always decrease with increasing distance, and in most cases (except when a very powerful $+I$ or $-I$ group is involved), cause very little difference in a bond four bonds away or more. There is evidence that field effects can be affected by the solvent.⁴⁹

For discussions of field effects on acid and base strength and on reactivity, see Chapters 8 and 9, respectively.

Bond Distances⁵⁰

The distances between atoms in a molecule are characteristic properties of the molecule and can give us information if we compare the same bond in different molecules. The chief methods of determining bond distances and angles are x-ray diffraction (only for solids), electron diffraction (only for gases), and spectroscopic methods, especially microwave spectroscopy. The distance between the atoms of a bond is not constant, since the molecule is always vibrating; the measurements obtained are therefore average values, so that different methods give different results.⁵¹ However, this must be taken into account only when fine distinctions are made.

Measurements vary in accuracy, but indications are that similar bonds have fairly constant lengths from one molecule to the next, though exceptions are known.⁵² The variation is generally less than 1%. Table 1.4 shows distances for single bonds between two sp^3 carbons.

⁴³For a review of field and other effects of silicon-containing groups, see Bassindale; Taylor, in Patai and Rappoport, Ref. 9, pp. 893-963.

⁴⁴For a review of the field effects of alkyl groups, see Levitt; Widing *Prog. Phys. Org. Chem.* 1976, 12, 119-157.

⁴⁵See Sebastian *J. Chem. Educ.* 1971, 48, 97.

⁴⁶See, for example, Schleyer; Woodworth *J. Am. Chem. Soc.* 1968, 90, 6528; Wahl; Peterson *J. Am. Chem. Soc.* 1970, 92, 7238. The situation may be even more complicated. See, for example, Minot; Eisenstein; Hiberty; Anh *Bull. Soc. Chim. Fr.* 1980, II-119.

⁴⁷Streitwieser; Klein *J. Am. Chem. Soc.* 1963, 85, 2759.

⁴⁸Bent *Chem. Rev.* 1961, 61, 275-311, p. 281.

⁴⁹See Laurence; Berthelot; Lucon; Helbert; Morris; Gal *J. Chem. Soc., Perkin Trans. 2* 1984, 705.

⁵⁰For tables of bond distances and angles, see Allen; Kennard; Watson; Brammer; Orpen; Taylor *J. Chem. Soc., Perkin Trans. 2* 1987, S1-S19; Tables of Interatomic Distances and Configurations in Molecules and Ions *Chem. Soc. Spec. Publ. No. 11*, 1958; Interatomic Distances Supplement *Chem. Soc. Spec. Publ. No. 18*, 1965; Harmony; Laurie; Kuczkowski; Schwendeman; Ramsay; Lovas; Lafferty; Maki *J. Phys. Chem. Ref. Data* 1979, 8, 619-721. For a review of molecular shapes and energies for many small organic molecules, radicals, and cations calculated by molecular orbital methods, see Lathan; Curtiss; Hehre; Lisle; Pople *Prog. Phys. Org. Chem.* 1974, 11, 175-261. For a discussion of substituent effects on bond distances, see Topsom *Prog. Phys. Org. Chem.* 1987, 16, 85-124.

⁵¹Burkert; Allinger *Molecular Mechanics*; ACS Monograph 177, American Chemical Society: Washington, 1982, pp. 6-9; Whiffen *Chem. Br.* 1971, 7, 57-61; Stals *Rev. Pure Appl. Chem.* 1970, 20, 1-22, pp. 2-5.

⁵²Schleyer; Bremer *Angew. Chem. Int. Ed. Engl.* 1989, 28, 1226 [*Angew. Chem.* 101, 1264].

TABLE 1.4 Bond lengths between sp^3 carbons in some compounds

C—C bond in	Bond length, Å	C—C bond in	Bond length, Å
Diamond ⁵³	1.544	Cyclohexane ⁵⁷	1.540 ± 0.015
C ₂ H ₆ ⁵⁴	1.5324 ± 0.0011	<i>t</i> -Butyl chloride ⁵⁸	1.532
C ₂ H ₅ Cl ⁵⁵	1.5495 ± 0.0005	<i>n</i> -Butane to <i>n</i> -heptane ⁵⁹	1.531–1.534
C ₃ H ₈ ⁵⁶	1.532 ± 0.003	Isobutane ⁶⁰	1.535 ± 0.001

However, an analysis of C—OR bond distances in more than 2000 ethers and carboxylic esters (all with sp^3 carbon) shows that this distance increases with increasing electron withdrawal in the R group and as the C changes from primary to secondary to tertiary.⁶¹ For these compounds, mean bond lengths of the various types ranged from 1.418 to 1.475 Å.

Bond distances for some important bond types are given in Table 1.5.⁶² As can be seen in this table, carbon bonds are shortened by increasing *s* character. This is most often explained by the fact that, as the percentage of *s* character in a hybrid orbital increases, the orbital becomes more like an *s* orbital and hence is held more tightly by the nucleus than an orbital with less *s* character. However, other explanations have also been offered (see p. 31), and the matter is not completely settled.

Indications are that a C—D bond is slightly shorter than a corresponding C—H bond. Thus, electron-diffraction measurements of C₂H₆ and C₂D₆ showed a C—H bond distance of 1.1122 ± 0.0012 Å and a C—D distance of 1.1071 ± 0.0012 Å.⁵⁴

Bond Angles

It might be expected that the bond angles of sp^3 carbon would always be the tetrahedral angle 109°28', but this is so only where the four groups are identical, as in methane, neopentane, or carbon tetrachloride. In most cases the angles deviate a little from the pure tetrahedral value. For example, the C—C—Br angle in 2-bromopropane is 114.2°.⁷⁰ Similarly, slight variations are generally found from the ideal values of 120 and 180° for sp^2 and sp carbon, respectively. These deviations occur because of slightly different hybridizations, that is, a carbon bonded to four other atoms hybridizes one *s* and three *p* orbitals, but the four hybrid orbitals thus formed are generally not exactly equivalent, nor does each contain exactly 25% *s* and 75% *p* character. Because the four atoms have (in the most general case) different electronegativities, each makes its own demand for electrons from the carbon atom.⁷¹ The carbon atom supplies more *p* character when it is bonded to more electronegative atoms, so that in chloromethane, for example, the bond to chlorine has somewhat more

⁵³Lonsdale *Phil. Trans. R. Soc. London* **1947**, A240, 219.

⁵⁴Bartell; Higginbotham *J. Chem. Phys.* **1965**, 42, 851.

⁵⁵Wagner; Dailey *J. Chem. Phys.* **1957**, 26, 1588.

⁵⁶Iijima *Bull. Chem. Soc. Jpn.* **1972**, 45, 1291.

⁵⁷Tables of Interatomic Distances, Ref. 50.

⁵⁸Momany; Bonham; Druehinger *J. Am. Chem. Soc.* **1963**, 85, 3075; also see Lide; Jen *J. Chem. Phys.* **1963**, 38, 1504.

⁵⁹Bonham; Bartell; Kohl *J. Am. Chem. Soc.* **1959**, 81, 4765.

⁶⁰Hilderbrandt; Wieser *J. Mol. Struct.* **1973**, 15, 27.

⁶¹Allen; Kirby *J. Am. Chem. Soc.* **1984**, 106, 6197; Jones; Kirby *J. Am. Chem. Soc.* **1984**, 106, 6207.

⁶²Except where noted, values are from Allen et al., Ref. 50. In this source, values are given to three significant figures.

⁶³Costain; Stoicheff *J. Chem. Phys.* **1959**, 30, 777.

⁶⁴For a full discussion of alkyne bond distances, see Simonetta; Gavezzotti, Ref. 7.

TABLE 1.5 Bond distances

The values given are average lengths and do not necessarily apply exactly to the compounds mentioned⁶²

Bond type	Length, Å	Typical compounds		
C—C				
sp^3-sp^3	1.53			
sp^3-sp^2	1.51	Acetaldehyde, toluene, propene		
sp^3-sp	1.47	Acetonitrile, propyne		
sp^2-sp^2	1.48	Butadiene, glyoxal, biphenyl		
sp^2-sp	1.43	Acrylonitrile, vinylacetylene		
$sp-sp$	1.38	Cyanoacetylene, butadiyne		
C=C				
sp^2-sp^2	1.32	Ethylene		
sp^2-sp	1.31	Ketene, allenes		
$sp-sp^{63}$	1.28	Butatriene, carbon suboxide		
C≡C⁶⁴				
$sp-sp$	1.18	Acetylene		
C—H⁶⁵				
sp^3-H	1.09	Methane		
sp^2-H	1.08	Benzene, ethylene		
$sp-H^{66}$	1.08	HCN, acetylene		
C—O				
sp^3-O	1.43	Dimethyl ether, ethanol		
sp^2-O	1.34	Formic acid		
C=O				
sp^2-O	1.21	Formaldehyde, formic acid		
$sp-O^{57}$	1.16	CO ₂		
C—N				
sp^3-N	1.47	Methylamine		
sp^2-N	1.38	Formamide		
C=N				
sp^2-N	1.28	Oximes, imines		
C≡N				
$sp-N$	1.14	HCN		
C—S				
sp^3-S	1.82	Methanethiol		
sp^2-S	1.75	Diphenyl sulfide		
$sp-S$	1.68	CH ₃ SCN		
C=S				
$sp-S$	1.67	CS ₂		
C—halogen⁶⁷	F	Cl	Br	I
$sp^3-halogen$	1.40	1.79	1.97	2.16
$sp^2-halogen$	1.34	1.73	1.88	2.10
$sp-halogen$	1.27 ⁶⁸	1.63	1.79 ⁶⁹	1.99 ⁶⁹

⁶²For an accurate method of C—H bond distance determination, see Henry *Acc. Chem. Res.* **1987**, *20*, 429-435.

⁶³Bartell; Roth; Hollowell; Kuchitsu; Young *J. Chem. Phys.* **1965**, *42*, 2683.

⁶⁴For reviews of carbon-halogen bonds, see Trotter, in Patai *The Chemistry of the Carbon-Halogen Bond*, pt. 1; Wiley: New York, 1973, pp. 49-62; Mikhailov *Russ. Chem. Rev.* **1971**, *40*, 983-997.

⁶⁵Lide, *Tetrahedron* **1962**, *17*, 125.

⁶⁶Rajput; Chandra *Bull. Chem. Soc. Jpn.* **1966**, *39*, 1854.

⁶⁷Schwendeman; Tobiasson *J. Chem. Phys.* **1965**, *43*, 201.

⁶⁸For a review of this concept, see Bingel; Lüttke *Angew. Chem. Int. Ed. Engl.* **1981**, *20*, 899-910 [*Angew. Chem.* **93**, 944-956].